Number Statistics of Ultracold Bosons in Optical Lattice

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(Dated: February 6, 2008)

We study the number statistics of ultracold bosons in optical Lattice using the slave particle technique and quantum Monte Carlo simulations. For homogeneous Bose-Hubbard model, we use the slave particle technique to obtain the number statistics near the superfluid to normal-liquid phase transition. The qualitatively behavior agree with the recent experiment probing number fluctuation [Phys. Rev. Lett. **96**, 090401 (2006)]. We also perform quantum Monte Carlo simulations to 1D system with external harmonic trap. The results qualitatively agree with the experiments.

PACS numbers: 03.75.Lm,67.40.-w,39.25.+k

I. INTRODUCTION

The ultracold atoms in optical lattices have opened a new windows to investigate the strongly correlated systems with highly tunable parameters[1]. The basic physics of these ultracold atoms is captured by the Bose Hubbard model, whose most fundamental feature is the existence of superfluid to Mott-insulator phase transition at zero temperature[2,3]. In a very shallow optical lattice, the ultracold bosons are in superfluid phase and can be well described by a macroscopic wave function with long-range phase coherence[4]. In this case, the phase fluctuation is zero and the on-site number fluctuation is large. When the optical lattice is very deep, the bosons enter the Mott-insulating phase with fixed number of atoms per site and without phase coherence, i.e., the on-site number fluctuation is zero and the phase fluctuation is large[4,5]. The physics of the MI phase is that, when the repulsive interaction between the atoms is large enough, the number fluctuation would become energetically unfavorable and the system would be in a number-squeezed state. This interaction induced MI phase plays an important role in the strongly correlated systems, as well as in various quantum information processing schemes[6].

In the past, some ultracold-atom experiments have been performed to detected these number-squeezed MI phase through the observation of increased phase fluctuations[4,5,7] or through an increased time scale for phase diffusion[8]. Recently, the continuous suppression of on-site number fluctuations was directly observed by Fabrice Gerbier et al by monitoring the suppression of spin-changing collisions across the superfluid/Mott-insulator transition[9]. By using a far off-resonant microwave field, the spin oscillations for doubly occupied sites can be tuned into resonance and the amplitude of spin oscillation is directly related to the probability of finding atom pairs per lattice site. It was shown by Fabrice Gerbier et al that, for small atom number, the oscillation amplitude is increasingly suppressed with increasing lattice depths and completely vanishes for large lattice depths. In the MI region, this suppression persists up to some threshold atom number. The authors also compared their experimental results with the prediction of the Bose Hubbard model within a mean-field approximation at zero temperature.

In this paper, we try to use the other approaches to study the number fluctuation beyond the zero-temperature mean-field theory. We first use the slave particle technique to obtained the number statistics at the critical points of the superfluid to normal liquid phase transition. The qualitative behaviors are the same as the recent experiment[9]. In the second part of this paper, we step out the mean-field theory and perform quantum Monte Carlo simulation to the 1D ultracold bosons with external harmonic trap. The numerical results reproduce the qualitative behaviors of the experiment.

This paper was organized as follows. In Sec. II, we will describe the slave particle technique to the homogeneous Bose-Hubbard model. In Sec. III, we will perform quantum Monte Carlo simulation to the 1D ultracold bosons with external harmonic trap. In Sec. IV, we will give our conclusions.

II. SLAVE-PARTICLE APPROACH TO THE NUMBER FLUCTUATION OF HOMOGENOUS BOSE-HUBBARD MODEL

We consider an ultracold atomic gas trapped in an three-dimensional optical lattice potential, $V_0(\mathbf{r}) = V_0\sum_{j=1}^{3}\sin^2(kr_j)$, with wave vectors $k = 2\pi/\lambda$ and λ the laser wavelength. In real experiments, an additional harmonic potential is superimposed to the lattice potential; however, we only pay attention to the homogeneous case in this section, which can be described by the following homogeneous Bose-Hubbard Hamiltonian[3],

$$H = -t\sum_{<ij>} a_i^\dagger a_j - \mu\sum_i n_i + \frac{U}{2}\sum_i n_i(n_i-1). \quad (1)$$

Here $a_i^\dagger$ is the creation operator at site i, $n_i = a_i^\dagger a_i$ is the particle number operator, and $\langle ij\rangle$ denotes the sum

over nearest neighbor sites. t and U are the hopping amplitude and on-site interaction, respectively,

$$t = \int d\mathbf{r} w^*(\mathbf{r}-\mathbf{r}_i)\left(-\frac{\hbar^2}{2m}\nabla^2 + V_0(\mathbf{r})\right) w(\mathbf{r}-\mathbf{r}_j),$$
$$U = g\int d\mathbf{r}|w(\mathbf{r})|^4. \qquad (2)$$

In the following, we will use the slave particle technique to obtain the finite temperature number fluctuation at the critical points. In the slave particle language[10,11], the bosonic creation operator $a_i^\dagger$ and annihilation operator a_i can be decomposed into

$$a_i^\dagger = \sum_{\alpha=0}\sqrt{\alpha+1}|\alpha+1\rangle_{ii}\langle\alpha|,$$
$$a_i = \sum_{\alpha=0}\sqrt{\alpha+1}|\alpha\rangle_{ii}\langle\alpha+1|, \qquad (3)$$

where $|\alpha\rangle_i$ is the eigenstate of the particle number operator $n_i = a_i^\dagger a_i$ with α the eigenvalue. In the slave particle language, every occupation state is identified as a type of slave particle, i.e., $|\alpha\rangle_i$ and ${}_i\langle\alpha|$ are mapped to $a_{\alpha,i}^\dagger$ and $a_{\alpha,i}$, which are the slave particle creation and annihilation operators, respectively. Then $a_i^\dagger$ and a_i can be rewritten as

$$a_i^\dagger = \sum_{\alpha=0}\sqrt{\alpha+1}a_{\alpha+1,i}^\dagger a_{\alpha,i},$$
$$a_i = \sum_{\alpha=0}\sqrt{\alpha+1}a_{\alpha,i}^\dagger a_{\alpha+1,i}. \qquad (4)$$

The slave particle operators are defined to satisfy the anticommutation relation $\{a_{\alpha,i}, a_{\beta,j}^\dagger\} = \delta_{\alpha\beta}\delta_{ij}$ in a slave fermion approach, and to satisfy the commutation relation $[a_{\alpha,i}, a_{\beta,j}^\dagger] = \delta_{\alpha\beta}\delta_{ij}$ in a slave boson approach. In order to reproduce the original bosonic commutation relation $[a_i, a_j^\dagger] = \delta_{ij}$, the slave particle operators must obey the constraint:

$$\sum_{\alpha=0} n_i^\alpha = \sum_{\alpha=0} a_{\alpha,i}^\dagger a_{\alpha,i} = 1. \qquad (5)$$

Substituting the slave particle transformation (4) into Eq. (1), the Bose-Hubbard Hamiltonian can be replaced by

$$H = -t\sum_{<ij>}\sum_{\alpha,\beta}\sqrt{\alpha+1}\sqrt{\beta+1}a_{\alpha+1,i}^\dagger a_{\alpha,i}a_{\beta,j}^\dagger a_{\beta+1,j}$$
$$-\mu\sum_i\sum_\alpha \alpha n_i^\alpha + \frac{U}{2}\sum_i\sum_\alpha \alpha(\alpha-1)n_i^\alpha. \qquad (6)$$

Following the steps in Refs.[12,13], we write the partition function as an imaginary time coherent state path integral[10,11]:

$$Z = \mathrm{Tr}e^{-\beta H} = \int Da_\alpha D\bar{a}_\alpha D\lambda e^{-S[\bar{a}_\alpha, a_\alpha, \lambda]}, \qquad (7)$$

$$S[\bar{a}_\alpha, a_\alpha, \lambda] = \int_0^\beta d\tau\Big[\sum_i\sum_\alpha \bar{a}_{\alpha,i}\Big(\partial_\tau - \alpha\mu + \frac{U}{2}\alpha(\alpha-1)$$
$$-i\lambda_i\Big)a_{\alpha,i} + i\sum_i\lambda_i$$
$$-t\sum_{<ij>}\sum_{\alpha,\beta}\sqrt{\alpha+1}\sqrt{\beta+1}\bar{a}_{\alpha+1,i}a_{\alpha,i}\bar{a}_{\beta,j}a_{\beta+1,j}\Big],$$
$$(8)$$

where $\bar{a}_{\alpha,i}$ and $a_{\alpha,i}$ are introduced as ordinary complex numbers in the slave boson approach, and as Grassmann variables in the slave fermion approach satisfying the Grassmann algebra. The Lagrange multiplier field $\lambda_i(\tau)$ comes from the constraint (5), namely, $\prod_i \delta(\sum_\alpha n_i^\alpha - 1)$. The unit has been set to $\hbar = k_B = 1$ in all formulas. In order to decouple the hopping term, we perform a Hubbard-Stratonovich transformation

$$\int D\Phi^* D\Phi \exp\Big[-\int d\tau t\sum_{<ij>}(\Phi_i^* - \sum_\alpha\sqrt{\alpha+1}\bar{a}_{\alpha+1,i}a_{\alpha,i})$$
$$\times(\Phi_j - \sum_\alpha\sqrt{\alpha+1}\bar{a}_{\alpha,j}a_{\alpha+1,j})\Big]. \quad (9)$$

The Hubbard-Stratonovich field Φ_i introduced here can be identified as the order parameter of superfluid for $\langle\Phi_i\rangle = \langle\sum_\alpha\sqrt{\alpha+1}\bar{a}_{\alpha,i}a_{\alpha+1,i})\rangle = \langle a_i\rangle$. We then perform a Fourier transform on all the fields A_i by

$$A_i = \frac{1}{\sqrt{L\beta}}\sum_{\mathbf{k},n}A_{\mathbf{k}n}e^{i(\mathbf{k}\cdot\mathbf{r}_i - \omega_n\tau)}, \qquad (10)$$

where L is the total number of sites of the optical lattice and ω_n is the Matsubara frequency, which equals $(2n+1)\pi/\beta$ or $2n\pi/\beta$ for fermionic or bosonic fields. After relaxing the constraint (5) to one slave particle per site on average over the whole lattice, i.e., replacing $\lambda_{\mathbf{k},n}$ with a constant $\lambda_{\mathbf{0},0}$, we arrive at an effective action divided into two parts,

$$S_{eff}[\Phi, a_\alpha, \lambda] = S_0 + S_I, \qquad (11)$$

$$S_0 = iL\beta\lambda + \sum_{\mathbf{k},n}\sum_\alpha \bar{a}_{\mathbf{k},n}^\alpha\left[-i\omega_n + c(\alpha)\right]a_{\mathbf{k},n}^\alpha$$
$$+ \sum_{\mathbf{k},n}\epsilon_{\mathbf{k}}|\Phi_{\mathbf{k},n}|^2 = S_0^{sp} + \sum_{\mathbf{k},n}\epsilon_{\mathbf{k}}|\Phi_{\mathbf{k},n}|^2,$$

$$S_I = -\sum_{\mathbf{k},\mathbf{k}',n,n'}\sum_\alpha\frac{\epsilon_{\mathbf{k}'}}{\sqrt{L\beta}}\Big[\Big(\sqrt{\alpha+1}\bar{a}_{(\mathbf{k}+\mathbf{k}'),(n+n')}^{\alpha+1}a_{\mathbf{k},n}^\alpha\Big)$$
$$\times\Phi_{\mathbf{k}',n'} + \Big(\sqrt{\alpha+1}\bar{a}_{\mathbf{k},n}^\alpha a_{(\mathbf{k}+\mathbf{k}'),(n+n')}^{\alpha+1}\Big)\Phi_{\mathbf{k}',n'}^*\Big],$$

where $c(\alpha) = -i\lambda - \alpha\mu + \alpha(\alpha-1)U/2$, $\lambda = \lambda_{\mathbf{0},0}/\sqrt{L\beta}$, and $\epsilon_{\mathbf{k}} = 2t\sum_{i=1}^d\cos(k_i a)$ with d and a being the dimension and spacing constant of the lattice.

Near the critical point, the order parameter Φ is small and the perturbation can be performed in terms of S_I. The partition function Z_0 of non-interacting slave particles comes from the contribution of the zeroth-order term S_0^{sp} which is given by

$$Z_0 = e^{-\beta\Omega_0} = \int Da_\alpha D\bar{a}_\alpha e^{-S_0^{sp}}. \tag{12}$$

Here Ω_0 is the zeroth-order thermodynamic potential,

$$-\Omega_0 = i\lambda L \pm \frac{L}{\beta}\sum_\alpha \ln(1 \pm e^{-\beta c(\alpha)}), \tag{13}$$

where the $+(-)$ sign corresponds to the slave fermion (slave boson). After expanding $e^{-S_{eff}}$ up to second order of S_I and integrating out the slave particle field, we obtain the new effective action to second order of the order parameter field,

$$S_{E,eff}[\Phi^*, \Phi] = \beta\Omega_0 - \sum_{\mathbf{k},n} \Phi^*_{\mathbf{k},n} G^{-1}(\mathbf{k}, i\omega_n)\Phi_{\mathbf{k},n}. \tag{14}$$

The Green's function $G(\mathbf{k}, i\omega_n)$ is defined by

$$-G^{-1}(\mathbf{k}, i\omega_n) = \epsilon_{\mathbf{k}} - \epsilon^2_{\mathbf{k}} \sum_\alpha (\alpha+1) \frac{n^\alpha - n^{\alpha+1}}{-i\omega_n - \mu + \alpha U}, \tag{15}$$

where n^α is the occupation number and equal to

$$n^\alpha = \frac{1}{\exp\{\beta[-i\lambda - \alpha\mu + \alpha(\alpha-1)U/2]\} \pm 1}, \tag{16}$$

in which the $+$ and $-$ sign correspond to slave fermion and slave boson, respectively.

The saddle point approximation to the constraint field λ means: $\partial\Omega/\partial\lambda = 0$; the particle number conservation condition requires $-\partial\Omega/\partial\mu = N$. The mean-field approximation means all the fluctuations coming from the Green's function would not be considered in the above two conditions. Then the following two mean-field equations can be derived,

$$\sum_{\alpha=0} n^\alpha = 1, \tag{17}$$

$$\sum_{\alpha=0} \alpha n^\alpha = \frac{N}{L} = n, \tag{18}$$

where the $n = N/L$ is the average particle density.

Combining Eqs. (15)-(18), we can obtain the number fluctuation at critical temperature of superfluid to normal liquid phase transition. We show the results in Fig.1. One can see that the qualitative behavior agree with the recent experiment probing number fluctuation [Phys. Rev. Lett. **96**, 090401 (2006)].

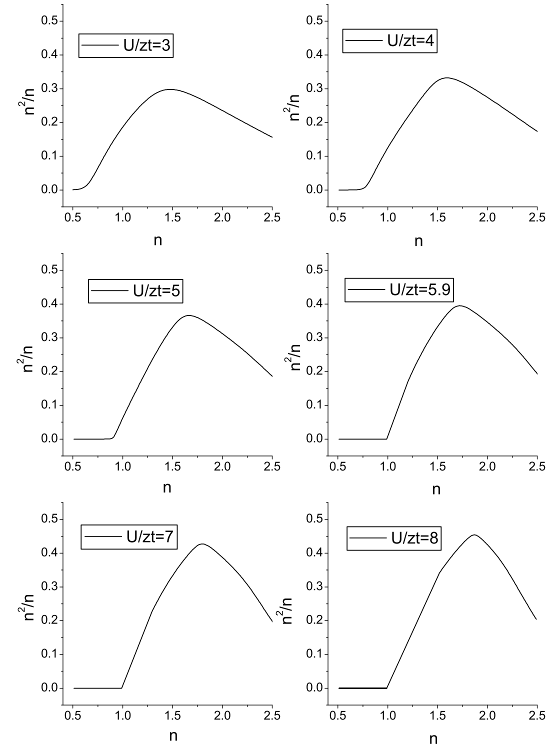

FIG. 1: The average probability of a site to be occupied by two bosons n^2/n as a function of average particle density n, for different interactions U/zt. All the calculations are performed at the critical temperature of the phase transition.

III. NUMERICAL RESULTS: QUANTUM MONTE CARLO CALCULATION IN ONE DIMENSION

Although mean field theory are applicable in higher dimensions, its application to 1D is questionable due to the large quantum fluctuations. In this section, we will come to the numerical calculation and focus our study on the Boson−Hubbard model (1) in a harmonic trapped potential in 1D optical lattice. The trapped potential we use is:

$$V_T = V_t \sum_i (i - L/2)^2 \tag{19}$$

where L is the chain length and $V_t = 0.02t$. The method we use is quantum Monte Carlo (QMC) simulations using the stochastic series expansion technique[14,15]. In the simulation, we set the lattice is large enough to neglect the boundary effects and the inverse of temperature $\beta = 100t$ in order to reach the ground state properties.

Fig.2 show $n_\alpha/\rho(\alpha = 1, 2, 3, 4)$ v.s. the average boson density ρ, where n_α is the average boson density for α bosons of the system. From the figure we can see, n_1 decreases with increasing average boson density ρ, while n_3, n_4 increase with it. They all change monotonously while n_2 is nonmonotonous. When ρ is small, n_1 is quite large, i.e., most of the sites are one particle occupied. In this region, there is a $n = 1$ Mott plateau in the middle of the chain(see fig.3). As ρ increases, n_1 decreases while n_2 increases slowly. At some critical ρ_{c1}, n_2 suddenly increases fast. This is because when $\rho > \rho_{c1}$, a superfluid

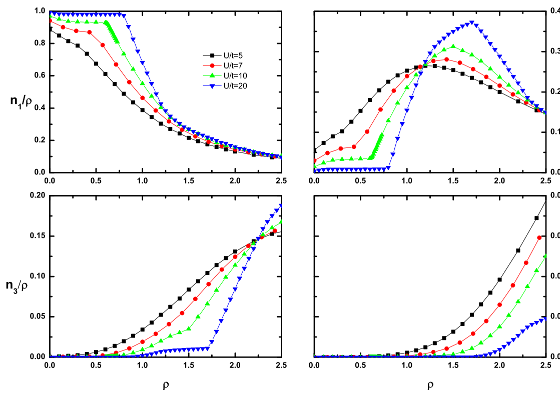

FIG. 2: (Color on line) n_α/ρ as a function of boson density ρ for various U/t at $V_t = 0.01t$. The chain size is $L = 100$. $n_\alpha(\alpha = 1, 2, 3, 4)$ are average bonson density for α bosons on each site.

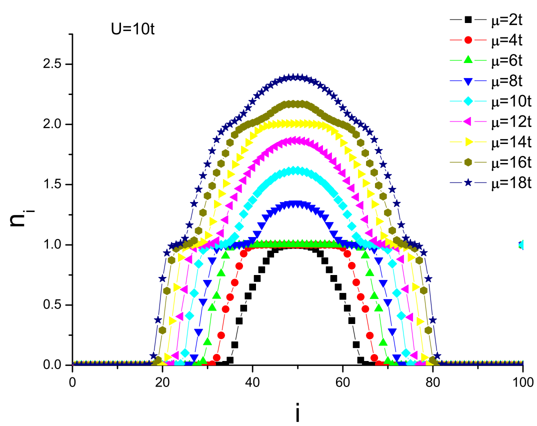

FIG. 3: (Color on line) Local particle density n_i as a function of site i for various μ at $U = 10t$.

forms in the middle of the $n = 1$ Mott plateau in the middle of the chain. As ρ increase further, n_2 reaches its maximum at ρ_{c2} and then decreases with increasing ρ. This corresponds the formation of the $n = 2$ Mott plateau in the middle of the chain(also see Fig.3). When U increase, both ρ_{c1} and ρ_{c2} increase. From the above discussion we can see that, n_2 can be used to describe the Mott-superfluid transition. Our results are qualitatively agree with Gerbier's experiment and the mean field theory above.

In Fig.3 and Fig.4, we show the local particle density and onsite number statistics for various μ at $U = 10t$. From Fig.3, we can see that the formation of the $n = 1$ and $n = 2$ plateau with increasing μ. In Fig.4 we find that n_1 develop concaves in the center of the trap. And these concaves become more and more deep which

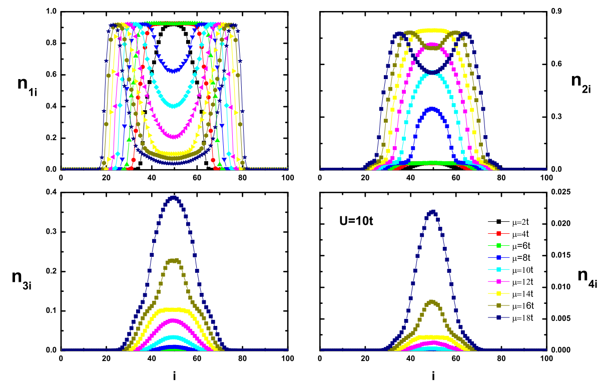

FIG. 4: (Color on line) n_α/ρ as a function of boson density ρ for various U/t at $V_t = 0.01t$. The chain size is $L = 100$. $n_\alpha(\alpha = 1, 2, 3, 4)$ are average bonson density for α bosons on each site.

correspond with the decreasing of the total number of n_1 in Fig.2. n_2 evolves nonmonotonously. It increase suddenly with the appearing of the superfluid region in the center of the trap and develop concave in the center of the trap with the appearing of the second Mott plateau. With the increasing of boson number, the n_3 and n_4 are not important when the total number of bosons are not large.

IV. CONCLUSION

We studied the number fluctuation of ultracold bosons in optical Lattice using the slave particle technique and quantum Monte Carlo simulation. By using the slave particle technique, we obtained the number statistic at the critical points of superfluid to normal liquid phase transition. We also performed QMC simulations to the one dimension Bose-Hubbard model with external harmonic trap. The numerical results qualitatively agree with the recent experiment[9].

Acknowledgments

This work was supported in part by Chinese National Natural Science Foundation. The simulations were performed on the HP-SC45 Sigma-X parallel computer of ITP and ICTS, CAS .

Note added.-Recently we became aware of a parallel numerical work[16] that reach similar conclusions.

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